

Optimal Numerical Differentiation Using Three Function Evaluations

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Abstract. Approximation of $f'(x)$ by a difference quotient of the form

$$h^{-1}[a_1 f(x + b_1 h) + a_2 f(x + b_2 h) + a_3 f(x + b_3 h)]$$

is found to be optimized for a wide class of real-valued functions by the surprisingly asymmetric choice of $\mathbf{b} = (b_1, b_2, b_3) = (1/\sqrt{3} - 1, 1/\sqrt{3}, 1/\sqrt{3} + 1)$. The nearly optimal choice of $\mathbf{b} = (-2, 3, 6)$ is also discussed.

1. Introduction. The problem of best approximating the derivative of a function at a single point using two values of the function is "best" solved by using the difference quotient

$$(1) \quad d_0(h) = \frac{f(x + \frac{1}{2}h) - f(x - \frac{1}{2}h)}{h}.$$

We consider the same problem using three values of the function and arrive at three different solutions by interpreting "best" in five different ways. Our best difference quotients are

$$(2) \quad d_1(h) = \frac{(3 - 2\sqrt{3})f\left(x + \left(\frac{1}{\sqrt{3}} + 1\right)h\right) + 4\sqrt{3}f\left(x + \frac{1}{\sqrt{3}}h\right) - (3 + 2\sqrt{3})f\left(x + \left(\frac{1}{\sqrt{3}} - 1\right)h\right)}{6h},$$

$$(3) \quad d_2(h) = \frac{f(x + h) + \omega^2 f(x + \omega h) + \omega f(x + \omega^2 h)}{3h},$$

where $\omega = -\frac{1}{2} + \sqrt{3}i/2$ and $\omega^2 = -\frac{1}{2} - \sqrt{3}i/2$ are the cube roots of 1, and

$$(4) \quad d_3(h) = \frac{32f(x + 3h) - 27f(x - 2h) - 5f(x + 6h)}{120h}.$$

Section 3 below was motivated by the kind suggestion of J. Lyness.

2. Minimum Truncation Error. Whenever we write f , we will mean either a complex-valued function of a complex variable or a real-valued function of a real variable. In the former case we assume that f is analytic near x and in the latter case that f is five times differentiable at x . The point x will be fixed and the variable h will be small. Our assumptions are chosen to guarantee (i) that f have at x a Taylor expansion to order h^4 with error $O(|h|^5)$ and (ii) that there be a bound for the modulus of f'''' near x .

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Consider the general three-point difference quotient

$$(5) \quad d(h) = h^{-1} \sum_{i=1}^3 a_i f(x + b_i h) = d(\mathbf{a}, \mathbf{b})(h).$$

Substituting Taylor's theorem,

$$f(x + b_i h) = \sum_{j=0}^4 \frac{f^{(j)}(x)}{j!} h^j b_i^j + \frac{f^{(5)}(\xi_i)}{5!} h^5 b_i^5,$$

into (5) and interchanging the order of summation gives

$$(6) \quad \begin{cases} d(h) = \sum_{j=0}^4 c_j \frac{f^{(j)}(x)}{j!} h^{j-1} + O(h^4), \\ c_j = \sum_{i=1}^3 a_i b_i^j, \quad j = 0, 1, 2, 3, 4. \end{cases}$$

For $d(h) \rightarrow f'(x)$ as $h \rightarrow 0$, we must have $c_0 = 0$ and $c_1 = 1$. This motivates our first definition.

Definition 1. A three-point rule for the first derivative is a difference quotient $d(\mathbf{a}, \mathbf{b})(h)$ of the form (5) where $c_0 = \sum a_i = 0$ and $c_1 = \sum a_i b_i = 1$.

Definition 2. A three-point rule for the first derivative is of degree k if and only if $d(\mathbf{a}, \mathbf{b})(h) = f'(0)$ for every polynomial f of degree k .

LEMMA 1. *A necessary and sufficient condition for the three-point rule to be of degree 3 is*

$$(7) \quad \begin{cases} c_0 = \sum a_i = 0, \\ c_1 = \sum a_i b_i = 1, \\ c_2 = \sum a_i b_i^2 = 0, \\ c_3 = \sum a_i b_i^3 = 0. \end{cases}$$

The proof of this is immediate from (6) above.

LEMMA 2. *No three-point rule is of degree 4. For a three-point rule to be degree 3, we must have all b_i distinct.*

Proof. For a rule to be of degree 4 would require $c_2 = c_3 = c_4 = 0$. Write this as a matrix equation

$$\mathbf{B}\mathbf{a} = \begin{pmatrix} b_1^2 & b_2^2 & b_3^2 \\ b_1^3 & b_2^3 & b_3^3 \\ b_1^4 & b_2^4 & b_3^4 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

If all $b_i \neq 0$, then the Vandermonde-like matrix B is nonsingular, so $\mathbf{a} = \mathbf{0}$, contrary to $c_1 = 1$. If, say, $b_3 = 0$, the three equations $c_2 = c_3 = 0$, $c_1 = 1$ lead quickly to a similar contradiction.

Similarly, if, say, $b_2 = b_3$, we may as well combine a_2 and a_3 , which implies we are dealing with a two-point rule. As above, if both $b_i \neq 0$, the two equations $c_2 = c_3 = 0$ force \mathbf{a} to be zero, contrary to $c_1 = 1$. The case of $b_2 = b_3 = 0$ is treated similarly. Thus, for a three-point rule to be of degree 3, we must have all b_i distinct.

LEMMA 3. The three-point rule d is of degree 3 if and only if

$$(8) \quad b_1 b_2 + b_1 b_3 + b_2 b_3 = 0.$$

Proof. The first three equations in (7), $c_0 = c_2 = 0$, $c_1 = 1$, may be written as a matrix equation

$$B\mathbf{a} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix},$$

where the Vandermonde matrix B is easily inverted. Substitute the result of this,

$$\mathbf{a} = [(b_2 - b_1)(b_3 - b_1)(b_3 - b_2)]^{-1}(b_2^2 - b_3^2, b_3^2 - b_1^2, b_1^2 - b_2^2),$$

into $c_3 = 0$ to obtain (8).

Definition 3. A three-point rule $d(\mathbf{a}, \mathbf{b})$ is said to be normalized if

$$\min\{|b_1 - b_2|, |b_1 - b_3|, |b_2 - b_3|\} = 1.$$

Motivation for Definition 3. The mapping $h \rightarrow ch$ for a nonzero constant c , which may also be thought of as mapping $(\mathbf{a}, \mathbf{b}) \rightarrow (c^{-1}\mathbf{a}, c\mathbf{b})$ while leaving h fixed, obviously does not change anything of substance. In other words, the set of three-point rules $d(\mathbf{a}, \mathbf{b})(h)$ partitions into equivalence classes with $d(\mathbf{a}, \mathbf{b}) \sim d(\mathbf{a}', \mathbf{b}')$ if there is a constant c such that $\mathbf{a}' = c^{-1}\mathbf{a}$ and $\mathbf{b}' = c\mathbf{b}$. The quantity $c_4(\mathbf{a}, \mathbf{b})$ is not a class invariant, for if $d(\mathbf{a}, \mathbf{b}) \sim d(\mathbf{a}', \mathbf{b}')$, where $(\mathbf{a}', \mathbf{b}') = (\varepsilon^{-1}\mathbf{a}, \varepsilon\mathbf{b})$ with $0 < \varepsilon < 1$, we have

$$(9) \quad |c_4(\mathbf{a}', \mathbf{b}')| = \left| \sum (\varepsilon^{-1}a_i)(\varepsilon b_i)^4 \right| = \varepsilon^3 |c_4(\mathbf{a}, \mathbf{b})| < |c_4(\mathbf{a}, \mathbf{b})|.$$

By picking ε very small, we can find arbitrarily small c_4 without really changing anything. Some normalization is required to keep the vector \mathbf{b} from collapsing to $\mathbf{0}$.

In difference quotient (1) or in the standard difference quotient $(f(x+h) - f(x))/h$, a normalization has been achieved by expressing the error in powers of the distance between the two arguments. Set

$$\delta = \min\{|b_1 - b_2|, |b_1 - b_3|, |b_2 - b_3|\}$$

and rewrite the dominant error term in (6) as

$$(10) \quad c_4 \frac{f^{(4)}(x)}{4!} h^3 = \left(\frac{c_4}{\delta^3} \right) \frac{f^{(4)}(x)}{4!} (\delta h)^3 = G \frac{f^{(4)}(x)}{4!} (\delta h)^3.$$

A simple calculation as in (9) above shows that $G = G(\mathbf{a}, \mathbf{b})$ is constant on each equivalence class.

LEMMA 4. All three-point rules of degree 3 are of the form

$$(11) \quad d(t) = \frac{t^3(t+2)f(x+(1+t)h) - (1+2t)f(x+t(1+t)h) - (t+1)^2(t^2-1)f(x-th)}{t(2t+1)(t+2)(t^2-1)h},$$

for some value of t , or are obtained from (11) by a transformation $(\mathbf{a}, \mathbf{b}) \rightarrow (c^{-1}\mathbf{a}, c\mathbf{b})$.

Proof. Select representatives from each equivalence class by setting $b_1 = 1$. Let $t = b_2$. From (8), $b_3 = -t/(t+1)$. Clear fractions by sending $(\mathbf{a}, \mathbf{b}) \rightarrow ((1/(t+1))\mathbf{a}, (t+1)\mathbf{b})$. Our representative quotient becomes (11).

THEOREM 1. *Let d be a normalized three-point rule of degree 3. Fix h and restrict \mathbf{a} and \mathbf{b} to be real. Then truncation error is minimized when $d = d_1$. (See Eq. (2).) This minimizing rule is unique up to the transformation $(\mathbf{a}, \mathbf{b}) \rightarrow (-\mathbf{a}, -\mathbf{b})$.*

Proof. Let $d'(\mathbf{a}', \mathbf{b}')$ be any normalized three-point rule of degree 3. By Lemma 1, we have $c_2(\mathbf{a}', \mathbf{b}') = c_3(\mathbf{a}', \mathbf{b}') = 0$, so to minimize truncation error we must minimize $|c_4(\mathbf{a}', \mathbf{b}')|$. By Lemma 4, there is a real number t and an equivalent three-point rule $d(t) = d(\mathbf{a}(t), \mathbf{b}(t))$ of the form (11). Since

$$|c_4(\mathbf{a}', \mathbf{b}')| = |c_4(\mathbf{a}', \mathbf{b}')/1^3| = |G(\mathbf{a}', \mathbf{b}')| = |G(\mathbf{a}, \mathbf{b})| = |c_4(\mathbf{a}, \mathbf{b})|/\delta^3,$$

where $\delta = \min_{i \neq j} \{|b_i - b_j|\}$ (see (10)), we see that we must minimize $|G(t)| = |c_4(\mathbf{a}(t), \mathbf{b}(t))|/\delta(\mathbf{b}(t))^3$ as t varies over \mathbf{R} .

Substituting the values of $\mathbf{a}(t)$ and $\mathbf{b}(t)$, as given in (11), into $|c_4(\mathbf{a}, \mathbf{b})|$ reduces our problem to that of minimizing

$$(12) \quad |G(t)| = \frac{|t^2(t+1)^2|}{\min\{|1-t^2|, |2t+1|, |t(t+2)|\}^3} = \frac{|t^2(t+1)^2|}{\delta(t)^3}.$$

Since t is real, we have

$$\delta(t) = \begin{cases} |t^2 - 1|, & -(\sqrt{3} + 1)/2 < t < -\sqrt{3} + 1, (\sqrt{3} - 1)/2 < t < \sqrt{3} + 1, \\ |t^2 + 2t|, & -(\sqrt{3} + 2) < t < -(\sqrt{3} + 1)/2, \sqrt{3} - 2 < t < (\sqrt{3} - 1)/2, \\ |2t + 1|, & -\infty < t < -(\sqrt{3} + 2), -\sqrt{3} + 1 < t < \sqrt{3} - 2, \sqrt{3} + 1 < t < \infty. \end{cases}$$

Substituting this into (12) and using the methods of elementary differential calculus on each interval yields that

$$\min_{t \in \mathbf{R}} |G(t)| = \frac{2}{9} \sqrt{3}$$

and that this minimum occurs at $t = 1 + \sqrt{3}, 1 - \sqrt{3}, \frac{1}{2}(\sqrt{3} - 1), \frac{1}{2}(-\sqrt{3} - 1), \sqrt{3} - 2$, and $-\sqrt{3} - 2$. All six values of t give equivalent difference quotients (the corresponding \mathbf{b} vectors are scalar multiples of one another). Normalizing the difference quotient corresponding to $t = \frac{1}{2}(\sqrt{3} - 1)$ by sending $(\mathbf{a}, \mathbf{b}) \rightarrow ((\sqrt{3}/2)\mathbf{a}, (2/\sqrt{3})\mathbf{b})$ produces difference quotient d_1 (see (2)) as the unique (up to $(\mathbf{a}, \mathbf{b}) \rightarrow (-\mathbf{a}, -\mathbf{b})$) normalized real three-point rule minimizing truncation error.

THEOREM 2. *Let d be a normalized three-point rule of degree 3. Fix h but allow all variables and functions to be complex-valued. Then truncation error is minimized when $d = d_2$. (See Eq. (3).) This minimizing rule is unique up to the transformations $(\mathbf{a}, \mathbf{b}) \rightarrow (e^{-i\varphi}\mathbf{a}, e^{i\varphi}\mathbf{b}), 0 < \varphi < 2\pi$.*

Proof. As in the proof of Theorem 1, we must minimize the function $|G(t)|$ given in (12). Since t may be complex,

$$(13) \quad \delta(t) = \begin{cases} |t^2 - 1| & \text{on } A_1, \\ |t^2 + 2t| & \text{on } A_2, \\ |2t + 1| & \text{on } A_3, \end{cases}$$

where A_1 is the union of the region enclosed by $C_1 \cup C_3$ with the region enclosed by $C_2 \cup C_4$, A_2 is the reflection of A_1 in the line $\operatorname{Re} t = -\frac{1}{2}$, and $A_3 = \mathbf{C} - (A_1 \cup A_2)$, where

$$C_1 = \left\{ -\frac{1}{2} + \frac{\sqrt{3}}{2} e^{i\theta}, 0 < |\theta| < \frac{\pi}{2} \right\},$$

$$C_2 = \left\{ -\frac{1}{2} + \frac{\sqrt{3}}{2} e^{i\theta}, \frac{\pi}{2} < |\theta| < \pi \right\},$$

$$C_3 = \left\{ 1 + \sqrt{3} e^{i\theta}, 0 < |\theta| < \frac{5}{6}\pi \right\},$$

$$C_4 = \left\{ 1 + \sqrt{3} e^{i\theta}, \frac{5}{6}\pi < |\theta| < \pi \right\}.$$

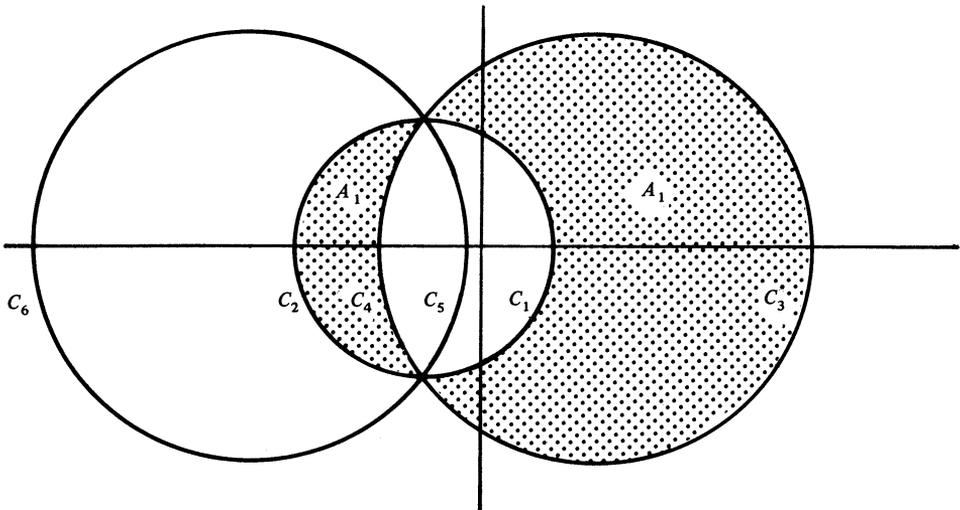


FIGURE 1

The shaded area in Figure 1 is A_1 . Substitute (13) into (12), use the maximum modulus theorem on $(G(t))^{-1}$ to see that the minimum of G must occur on one of the three circles of Figure 1, and use the method of elementary calculus on each circle, treating G as the appropriate function of θ on each C_i . The result is

$$\min_{t \in \mathbf{C}} |G(t)| = \frac{1}{9} \sqrt{3}$$

and that the minimum occurs at $t = \omega$ and ω^2 . Again, the corresponding difference quotients are equivalent; in fact, both are equivalent to difference quotient d_2 (see (3)). Notice that, for any nonzero complex constant $c = \rho e^{i\phi}$, the mapping $(\mathbf{a}, \mathbf{b}) \rightarrow (c^{-1}\mathbf{a}, c\mathbf{b})$, gives an equivalent best complex three-point rule minimizing truncation error. Thus the "obvious" best three-point rule here is any one obtained by letting \mathbf{b} be the three vertices of any equilateral triangle centered at x . (The word "obvious" is in quotes since the corresponding symmetric choice was not the best one in the real case above.)

3. Roundoff Error.

Motivation for Theorem 3. In the previous section, evaluations were assumed to be exact. Here we assume that each computation of the function f may be in error

by as much as $\pm \epsilon$ where ϵ is a small fixed positive quantity. From (5), we see that this generates a roundoff error bounded by

$$E_R = \frac{(|a_1| + |a_2| + |a_3|)\epsilon}{h} = \frac{A\epsilon}{h}.$$

Fix a difference quotient satisfying (7). From (6) and (7), we see that the dominant term in the truncation error is $c_4 f^{(4)}(x)(4!)^{-1}h^3$ which is dominated by

$$(14) \quad E_T = \frac{|c_4|f_4h^3}{4!},$$

where $f_4 = \sup\{|f^{(4)}(y)| : y \text{ is near } x\}$. Define the overall error E by $E = E_T + E_R$. Elementary calculus shows the h which makes E smallest to be given by

$$(15) \quad \begin{cases} h = \left(\frac{8A\epsilon}{|c_4|f_4} \right)^{1/4}, & \text{for which } h \text{ we have} \\ E = \frac{2^{5/4}}{3} (A^3|c_4|)^{1/4} f_4^{1/4} \epsilon^{3/4}. \end{cases}$$

THEOREM 3. *Let d be a normalized three-point rule of degree 3. Fix h and restrict \mathbf{a} and \mathbf{b} to be real. Then overall error is minimized when $d = d_1$. (See Eq. (2).) This minimizing rule is unique up to the transformation $(\mathbf{a}, \mathbf{b}) \rightarrow (-\mathbf{a}, -\mathbf{b})$.*

Proof. From (15) it follows that we have to minimize $A^3|c_4|$. (Note that $(\mathbf{a}, \mathbf{b}) \rightarrow (c^{-1}\mathbf{a}, c\mathbf{b})$ sends $A \rightarrow |c|A$, $|c_4| \rightarrow |c|^{-3}|c_4|$, so that this quantity is constant over each equivalence class.)

Assume \mathbf{a}, \mathbf{b} , and t are real. Then

$$\begin{aligned} A^3|c_4| &= \left(\sum |a_i| \right)^3 \left| \sum a_i b_i^4 \right| \\ &= \left(\frac{|t^3(t+2)| + |2t+1| + |(t+1)^2(t^2-1)|}{|t(2t+1)(t+2)(t^2-1)|} \right)^3 t^2(t+1)^2 \\ &= \begin{cases} 8t^8/|(t+1)[(2t+1)(t-1)]^3|, & -1 \leq t \leq -\frac{1}{2}, 1 \leq t < \infty, \\ 8(t+1)^8/|t[(2t+1)(t+2)]^3|, & -\infty < t \leq -2, -\frac{1}{2} \leq t \leq 0, \text{ and} \\ 8/|t(t+1)[(t+2)(t-1)]^3|, & -2 \leq t \leq -1, 0 \leq t < 1. \end{cases} \end{aligned}$$

By elementary calculus we have

$$\min_{t \in \mathbf{R}} A^3|c_4| = \left(\frac{2}{3} \right)^3 \cdot 2^4$$

and that this minimum occurs at $t = 1 + \sqrt{3}, 1 - \sqrt{3}, \frac{1}{2}(\sqrt{3} - 1), \frac{1}{2}(-\sqrt{3} - 1), \sqrt{3} - 2$, and $-\sqrt{3} - 2$. Thus rule d_1 also minimizes the overall error E among all real normalized three-point rules.

THEOREM 4. *Let d be a normalized three-point rule of degree 3. Fix h but allow all variables and functions to be complex-valued. Then overall error is minimized when $d = d_2$. (See Eq. (3).) This minimizing rule is unique up to the transformations $(\mathbf{a}, \mathbf{b}) \rightarrow (e^{-i\varphi}\mathbf{a}, e^{i\varphi}\mathbf{b}), 0 < \varphi < 2\pi$.*

Proof. Let $z = 2t + 1$. As in the proof of Theorem 3, we must minimize $A^3|c_4| = F(z)$ where

$$(16) \quad F(z) = \frac{1}{16} \left(\frac{|z-1|^3|z+3| + 16|z| + |z+1|^3|z-3|}{|z(z^2-9)|} \right)^3 \frac{1}{|z^2-1|}.$$

Inspired by the results of Section 2 (see Theorem 2), we were able to guess that the minimum would occur for $t = \omega$ and ω^2 , which correspond to $z = \sqrt{3}i$ or $z = -\sqrt{3}i$, where $F = 1$. Because of the symmetries $F(z) = F(\bar{z}) = F(-z)$, it suffices to show that $F > 1$ at every point of the first quadrant, C_+ , except $\sqrt{3}i$. Let $r = |z|$. For $z \in C_+$ and $a \geq 0$, we have $|z+a| \geq r$, so, from (16),

$$F(z) \geq \frac{1}{16} \left(\frac{(r-1)^3r + 16r + r^3(r-3)}{r(r^2+9)} \right)^3 \frac{1}{r^2+1} = g(r).$$

Direct calculation shows $g' > 0$ on $[9, \infty)$ and $g(9) > 1$, reducing the domain of investigation to $C_+ \cap \{|z| \leq 9\} = D$. Finally, a combination of evaluating F on the points of a mesh containing D , together with bounding $\text{grad } F$ away from the singularities $z = 0, 1, 3$, shows $F > 1$ away from $\sqrt{3}i$, while a Taylor expansion of F about $\sqrt{3}i$ shows $F > 1$ on the remainder of $D \setminus \{\sqrt{3}i\}$. Thus three-point rule d_2 also minimizes the overall error E among all normalized three-point rules.

4. A Third Rule and Some Remarks.

Motivation for the Third Rule (see (4)). Estimating the first derivative from an equally spaced table adds the constraint that all three b_i be integers. Under these conditions it is clear from formula (11) that the rule given by (4) is best in a number of ways. It is best among integer three-point rules of degree 3 with respect to (i) minimizing $\max\{b_i\} - \min\{b_i\}$, (ii) minimizing $\sum b_i^2$, (iii) minimizing $\sum |b_i|$, et cetera.

History of Three-Point Rules. Essentially all real three-point rules appearing in the literature have been only of degree 2. (However, compare [3, p. 217].) The most prevalent of these is $(-3f(x) + 4f(x+h) - f(x+2h))/2h$; see [1]. The complex rule (with $\mathbf{b} = (1, \omega, \omega^2)$) seems to be well known; see [2].

Comparison of Three-Point Rules. In Table 1 below, f_4 is a bound for the modulus of the fourth derivative near x . All derivatives have been normalized to make $\min|b_i - b_j| = 1$.

Observe that the overall error for the rule d_3 is only slightly worse than that of the rule d_1 . (By Theorem 3 it must be worse.)

Generalizations. 1. If we use $p > 3$ points in our approximating rule, the most we can hope to achieve is

$$(17) \quad c_1 = 1, \quad c_0 = c_2 = \cdots = c_p = 0.$$

This follows from a simple linear algebra argument like the one found in Lemma 2. Such a difference quotient is easily found in the complex case by letting \mathbf{b} be the p th roots of unity and solving the Vandermonde system,

$$c_1 = 1, \quad c_0 = c_2 = \cdots = c_{p-1} = 0,$$

for **a**. Such a quotient appears in [2]. The last equation in (17) holds automatically from the p -periodicity. The same result holds in the real case. If p is even, one simply finds the appropriate linear combination of $f(x + h) - f(x - h)$, $f(x + 2h) - f(x - 2h)$, \dots , $f(x + ph/2) - f(x - ph/2)$. This process is essentially Romberg extrapolation. If p is odd, more delicate arguments are required, but Eqs. (17) can still be satisfied.

TABLE I

$\begin{matrix} \text{a} \\ \text{-----} \\ \text{b} \end{matrix}$	Truncation Error (see (14))	Overall Error (see (15))
$\begin{matrix} 1 & & -1 \\ \text{-----} \\ 1/2 & & -1/2 \end{matrix}$ (see (1))	$\frac{f_3 h^2}{3!} \doteq .167 f_3 h^2$	$\frac{1}{2} 3^{2/3} f^{1/3} \epsilon^{2/3} \doteq 1.04 f_3^{1/3} \epsilon^{2/3}$
$\begin{matrix} \frac{3-2\sqrt{3}}{6} & \frac{4\sqrt{3}}{6} & \frac{-3-2\sqrt{3}}{6} \\ \text{-----} \\ \frac{1}{\sqrt{3}} + 1 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} - 1 \end{matrix}$ (see (2))	$\frac{2}{9} \sqrt{3} \frac{f_4}{4!} h^3 \doteq .016 f_4 h^3$	$\frac{8}{3^{7/4}} f_4^{1/4} \epsilon^{3/4} \doteq 1.17 f_4^{1/4} \epsilon^{3/4}$
$\begin{matrix} \frac{1}{\sqrt{3}} & \frac{\omega^2}{\sqrt{3}} & \frac{\omega}{\sqrt{3}} \\ \text{-----} \\ \frac{1}{\sqrt{3}} & \frac{\omega}{\sqrt{3}} & \frac{\omega^2}{\sqrt{3}} \end{matrix}$ (see (3))	$\frac{1}{9} \sqrt{3} \frac{f_4}{4!} h^3 \doteq .008 f_4 h^3$	$\frac{2^{5/4}}{3} f_4^{1/4} \epsilon^{3/4} \doteq .793 f_4^{1/4} \epsilon^{3/4}$
$\begin{matrix} \frac{32}{40} & & \frac{-27}{40} & & \frac{-5}{40} \\ \text{-----} \\ \frac{3}{3} & & \frac{-2}{3} & & \frac{6}{3} \end{matrix}$ (see (4))	$\frac{4}{3} \cdot \frac{f_4}{4!} h^3 \doteq .056 f_4 h^3$	$\frac{16}{3(375)^{1/4}} f_4^{1/4} \epsilon^{3/4} \doteq 1.21 f_4^{1/4} \epsilon^{3/4}$

2. Pass now to the d th derivative, $d \geq 2$. To approximate $f^{(d)}(x)$ we now need $p \geq d + 1$. As above, we choose **(a, b)** in such a way that $d(h)$ is an approximation to the d th derivative, i.e., that $c_0 = c_1 = \dots = c_{d-1} = 0$, $c_d = d!$ (see (6)) and that as many higher order terms be 0 as possible. Again the kind of argument used in Lemma 2 shows that we may hope for $c_{d+1} = c_{d+2} = \dots = c_{d+p-1} = 0$ at most. As in the preceding generalization 1, we may achieve this in the complex case by letting the components of **b** be the p th roots of unity. In the real case, however, we *cannot* always do as well. For example, let $d = 2$ and $p = 3$. Here

$$\frac{2}{3} [f(x + h) + \omega f(x + \omega h) + \omega^2 f(x + \omega^2 h)] / h^2 = f''(x) + \frac{1}{60} f^{(5)}(x) h^3 \dots$$

so $c_0 = c_1 = c_3 = c_4 = 0$, $c_2 = 2$, as desired, while an easy calculation shows this system to be insoluble with **a** and **b** real.

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